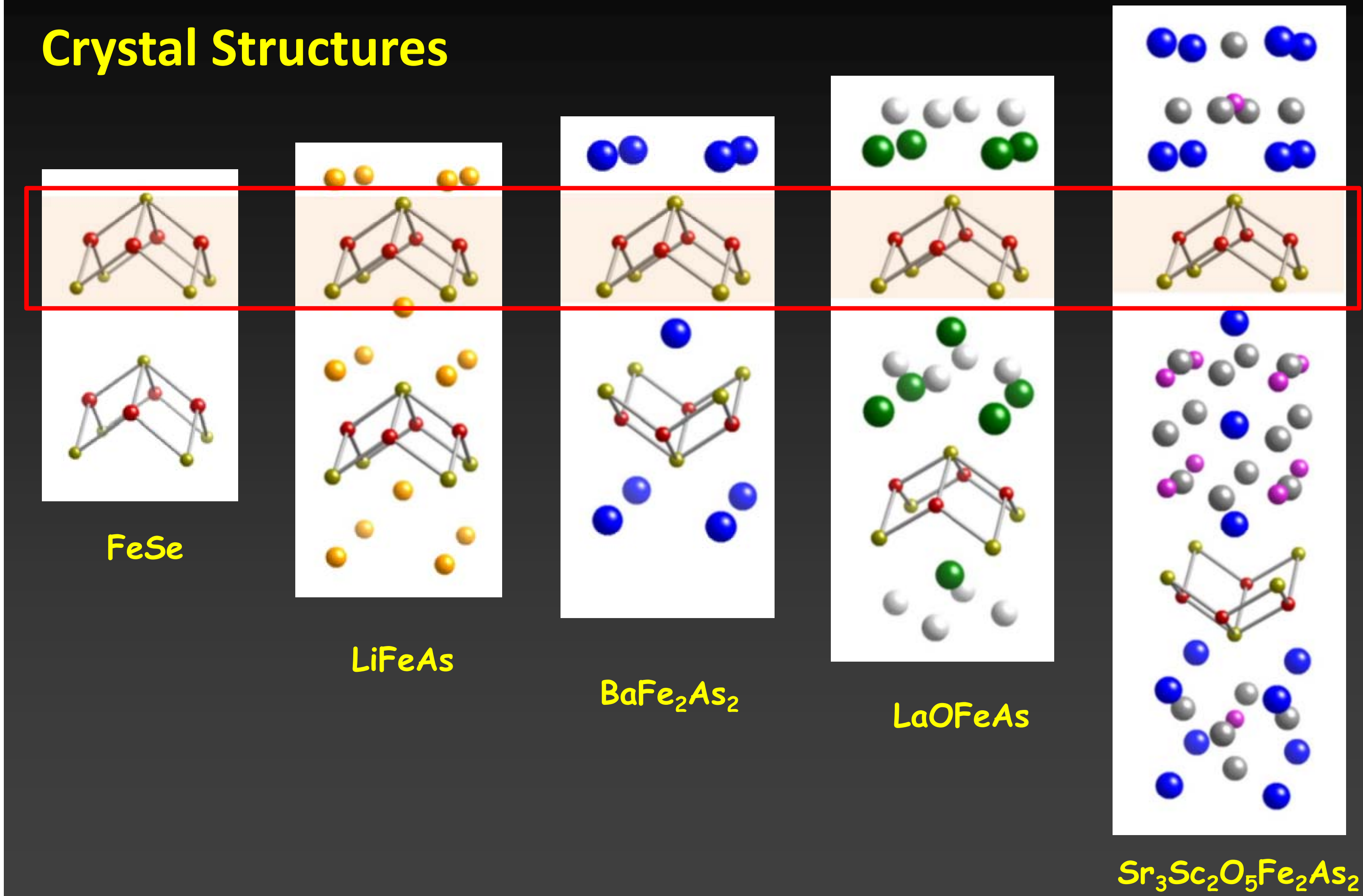
Luca de' Medici

(LPEM ESPCI - ParisTech)

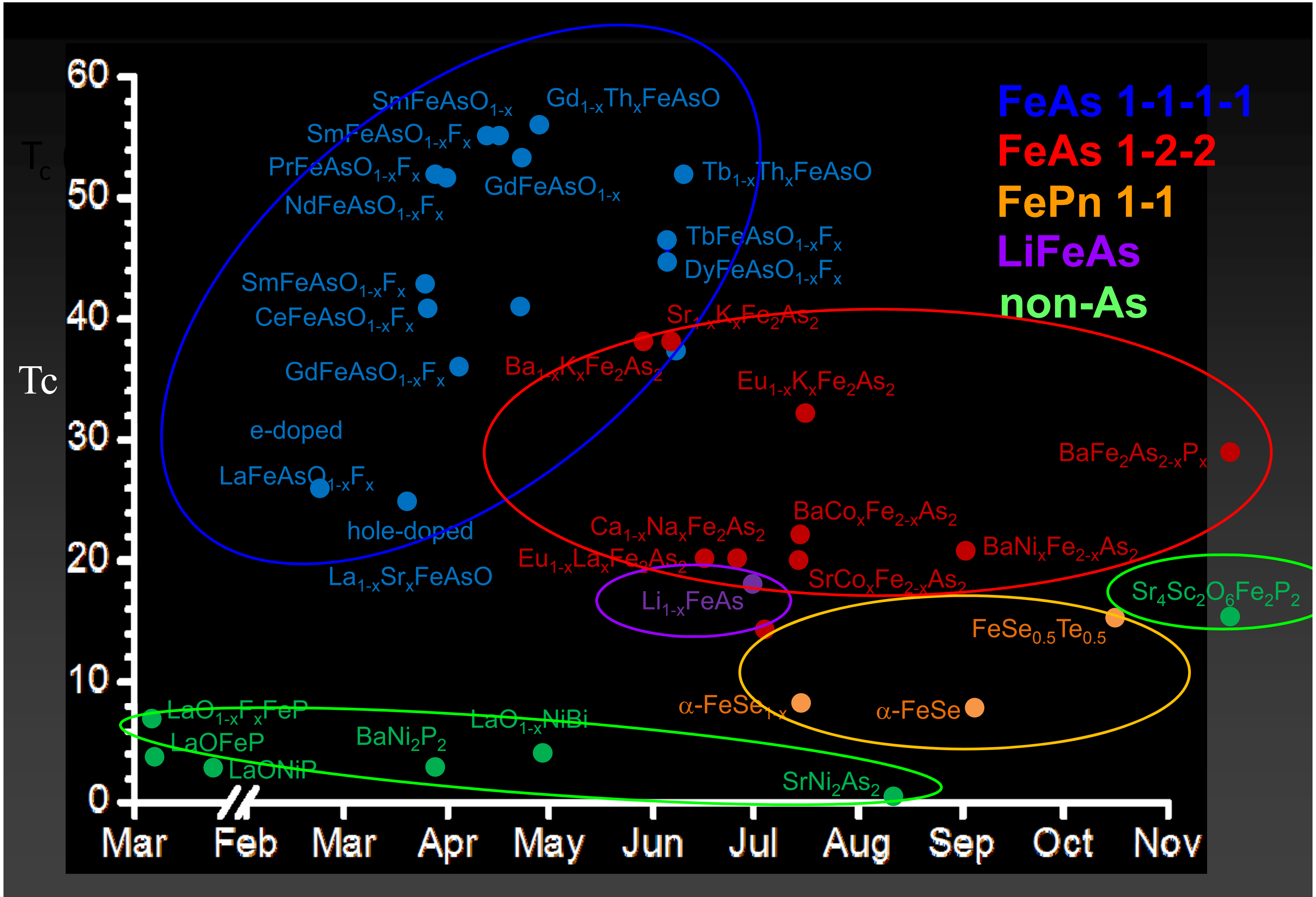
Selective Mottness as a key to iron superconductors

International workshop on
Recent developments in Fe-based high-temperature superconductors
Riverhead, NY 06.09.2013

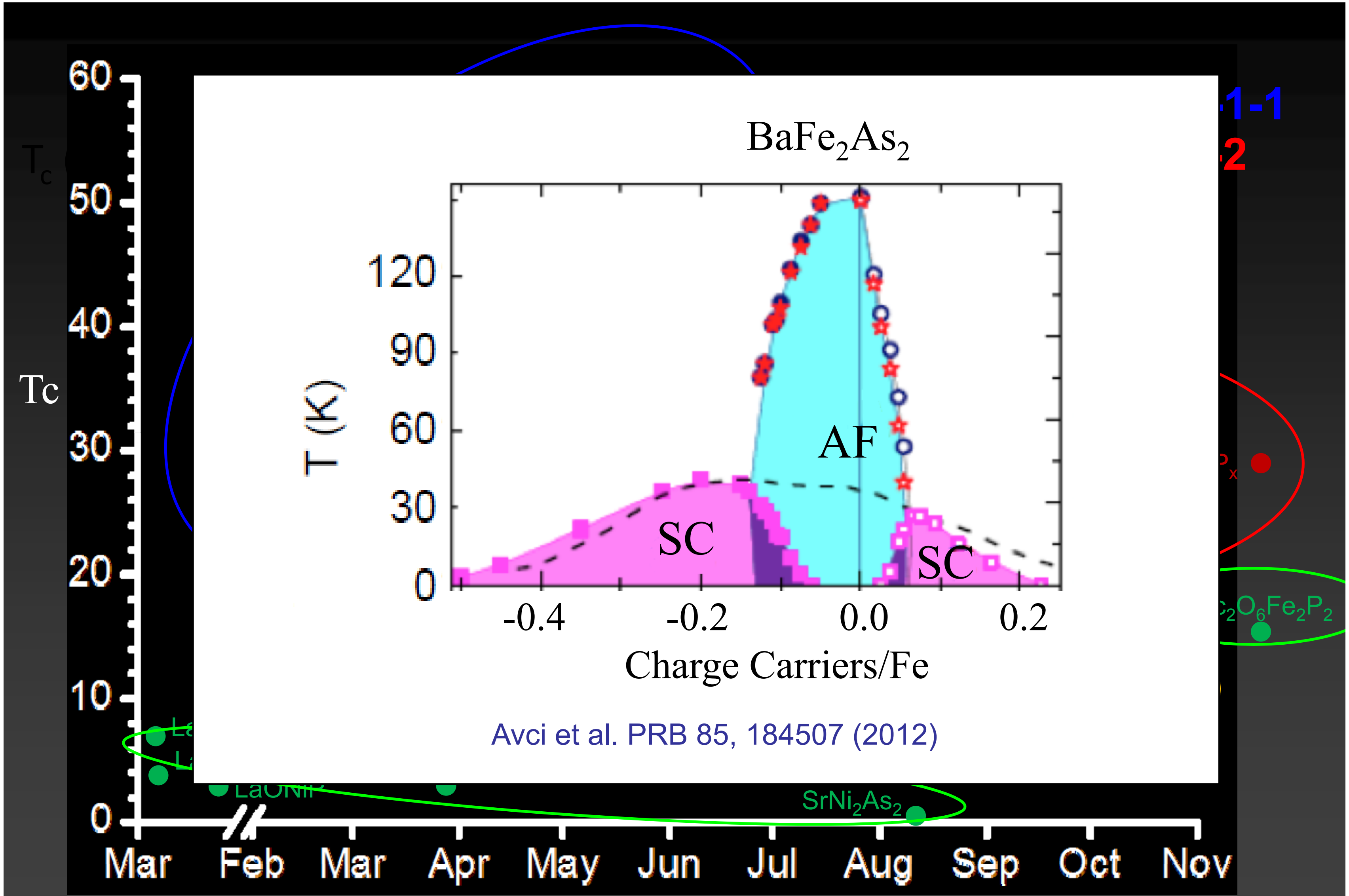
Crystal Structures



Paglione/Greene review (2010)



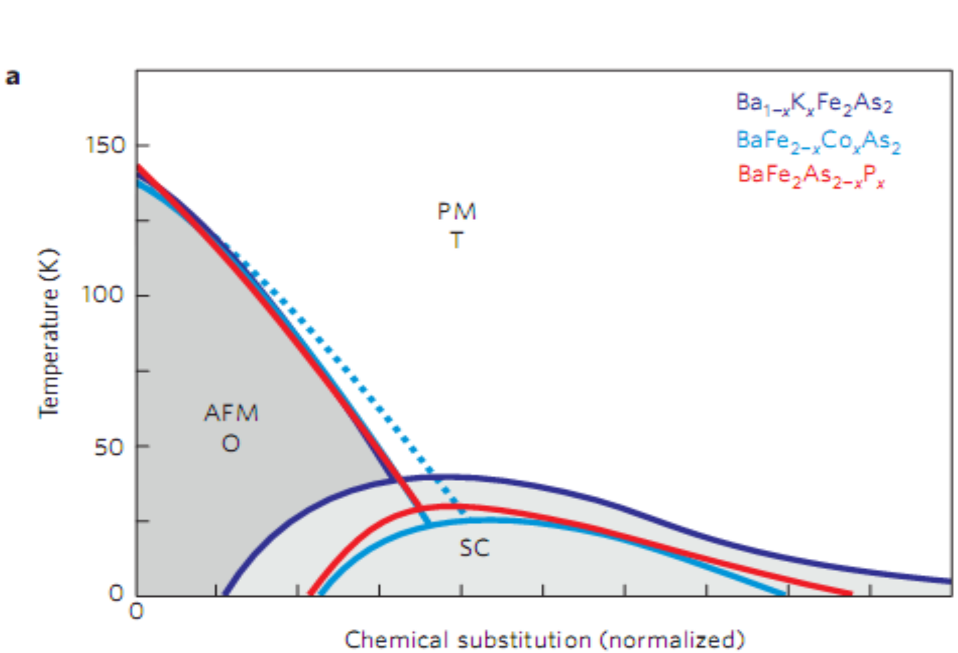
courtesy of J. Hoffman!

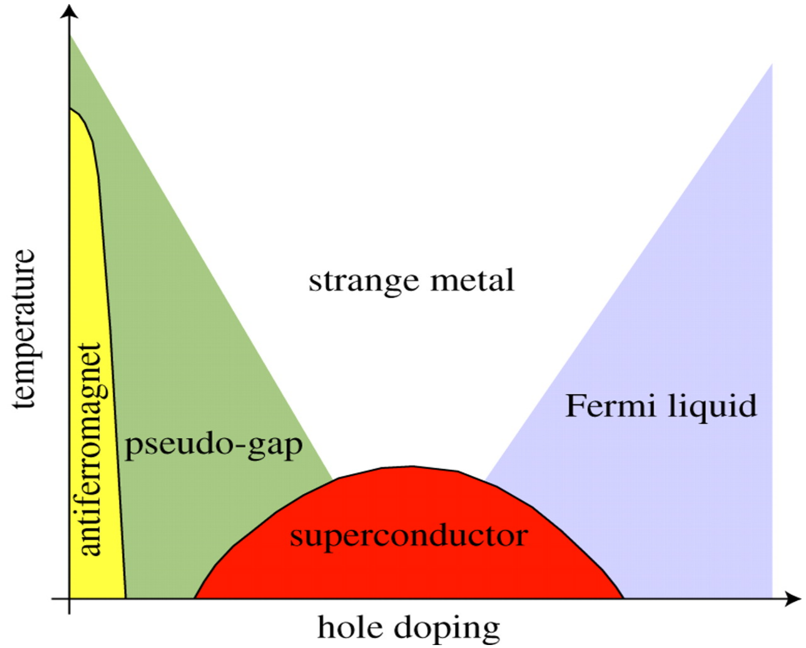


courtesy of J. Hoffman!

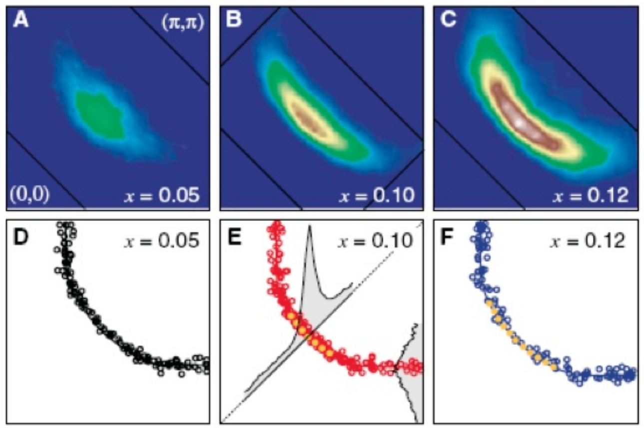
Analogies with Cuprates

Luca de' Medici

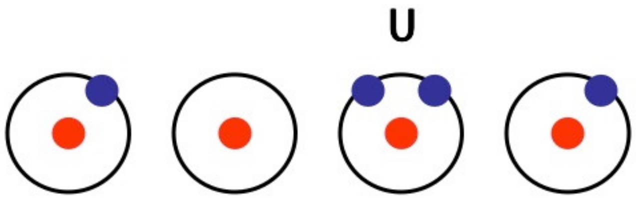




Big difference:
<u>no Mott insulator?!</u>



K. Shen et al.
Science 2007



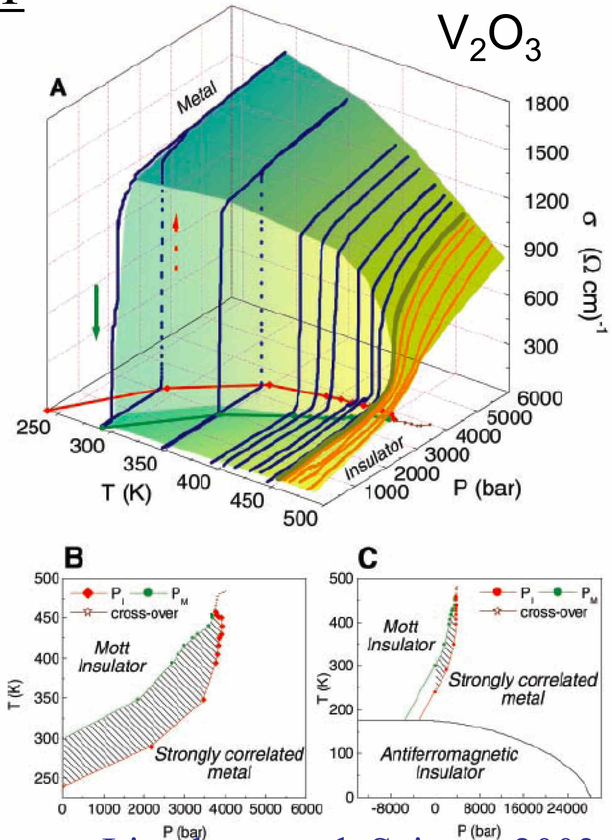
independent electrons → <u>Fermi liquid</u>

- Effective mass
- coherence Temperature
- U very strong ($U>U_c$): Mott Insulator

<u>Mott insulators are predicted metallic by DFT</u>

electrons are localized by correlations

(V_2O_3, Fullerenes, Cuprates…)

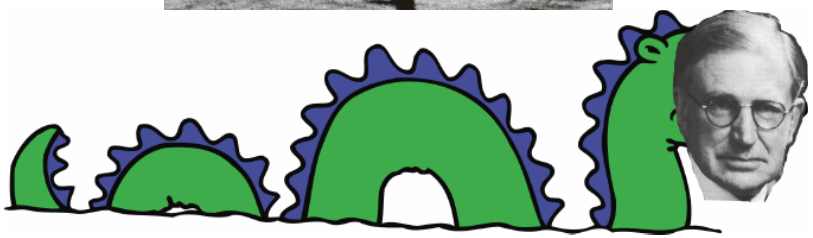


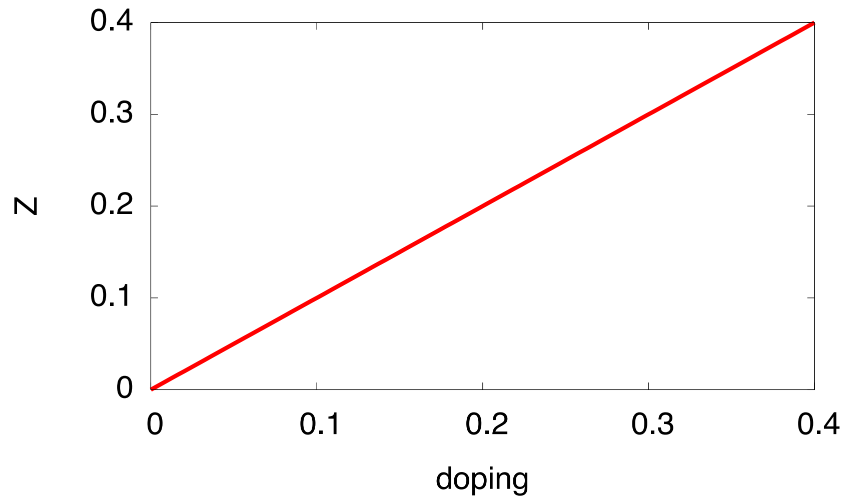
Limelette et al. Science 2003

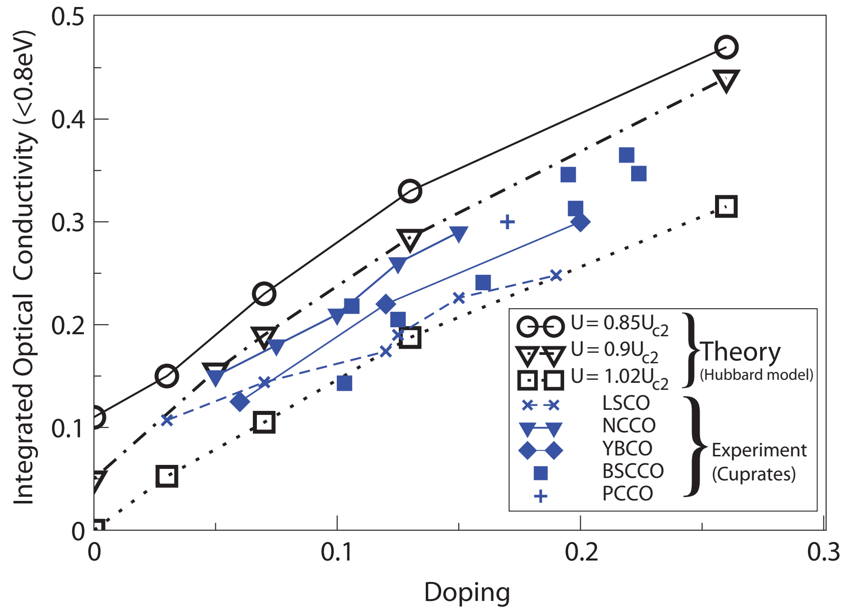
<u>The proximity to a Mott state strongly affects the properties of a system:</u>

- reduced metallicity (Z~x)
- mass enhancement
- transfer of spectral weight from low to high energy (e.g. in optical response)
- tendency towards magnetism
- …

'Mottness'







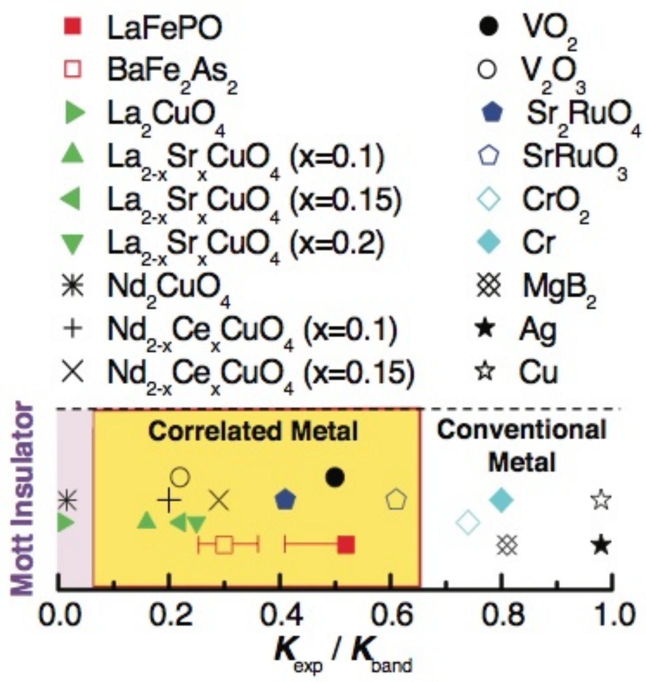
Comanac et al. NatPhys 2008

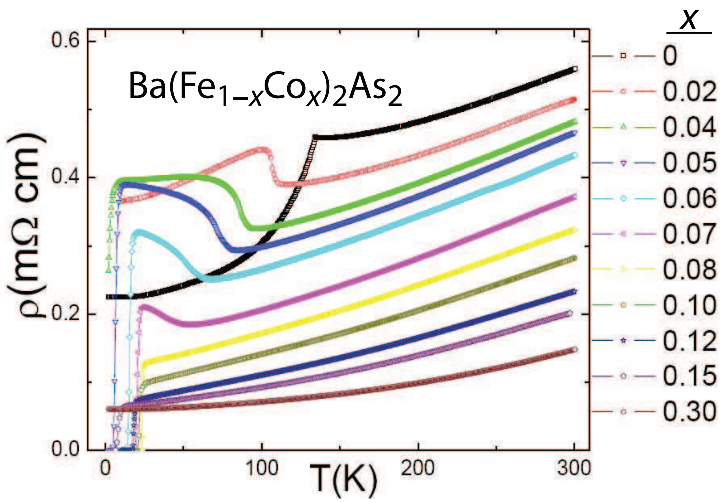
Contrasting evidences for correlation strenghts

- no Mott insulator in the phase diagram
- no detection of Hubbard bands
- moderate correlations from Optics
- bad metallicity
- strong sentitivity to doping
- local vs itinerant magnetism

<u>Weak-coupling vs Strong-coupling scenarios</u>

Qazilbash et al. NatPhys2009



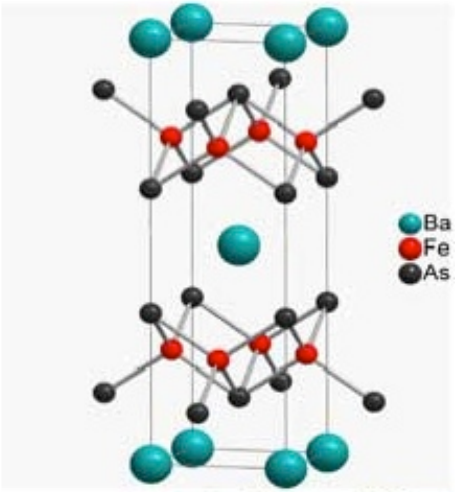


Fang et al. PRB80 (2009)

Specific heat (mJ/ mol K^2)

LaFePO	7
$Ba(Co_xFe_{1-x})_2As_2$	15-20
$Ba_{1-x}K_xFe_2As_2$	50
$FeSe_{0.88}$	9.2
KFe_2As_2	69-102
$K_{0.8}Fe_{1.6}Se_2$	6

Review: Stewart, RMP2011



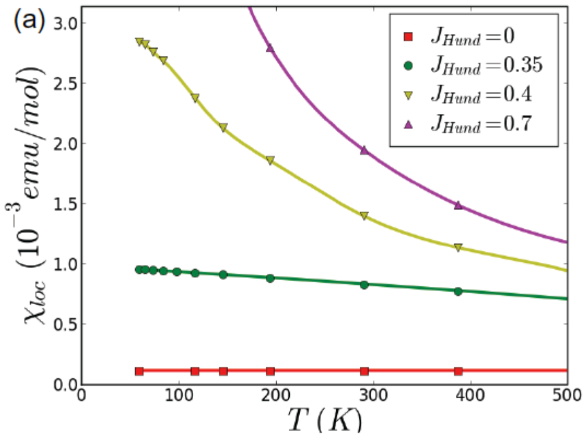
$BaFe_2As_2$

- cubic
- 5 bands (Fe 3d) at the Fermi level n=6 electrons
- Strong Hund's coupling J

- Partially lifted degeneracy

Theory:
'Hund's metals'

Haule and Kotliar, NJP 11 (2009)



$$H = \sum_k H_k^{DFT}$$

$$+U\sum_{i,m} n_{im\uparrow}n_{im\downarrow} + (U' - \frac{J}{2})\sum_{i,m>m'} n_{im}n_{im'}$$

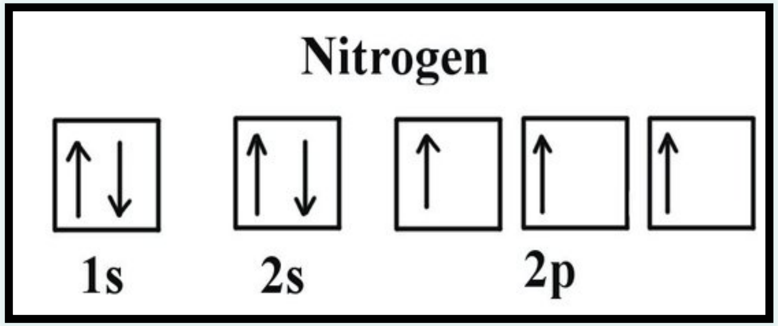
$$-J\sum_{i,m>m'}\Big[2\mathbf{S}_{im}\cdot\mathbf{S}_{im'} + (d^\dagger_{im\uparrow}d^\dagger_{im\downarrow}d_{im'\uparrow}d_{im'\downarrow} + h.c.)\Big]$$

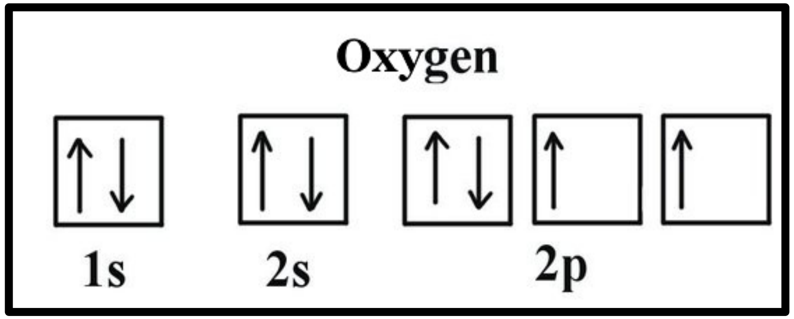
U'=U-2J

Hund's rules: atoms

Luca de' Medici

Aufbau





<u>Hund's Rules</u>

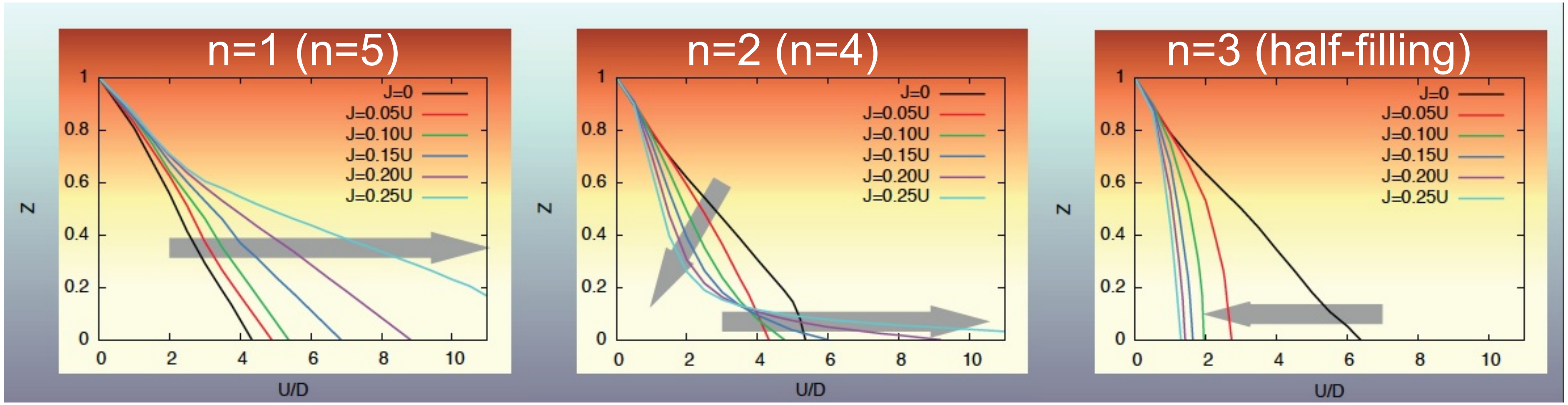
In open shells:

1. Maximize total spin S
2. Maximize total angular momentum T

(3. Dependence on J=T+S, Spin-orbit effects)

$$H_{\text{int}} = (U - 3J)\frac{\hat{N}(\hat{N}-1)}{2} - 2J\vec{S}^2 - \frac{1}{2}J\vec{T}^2$$

3 orbitals (relevant for t_{2g} materials)



Mott Gap: E(n+1)+E(n-1)-2E(n)

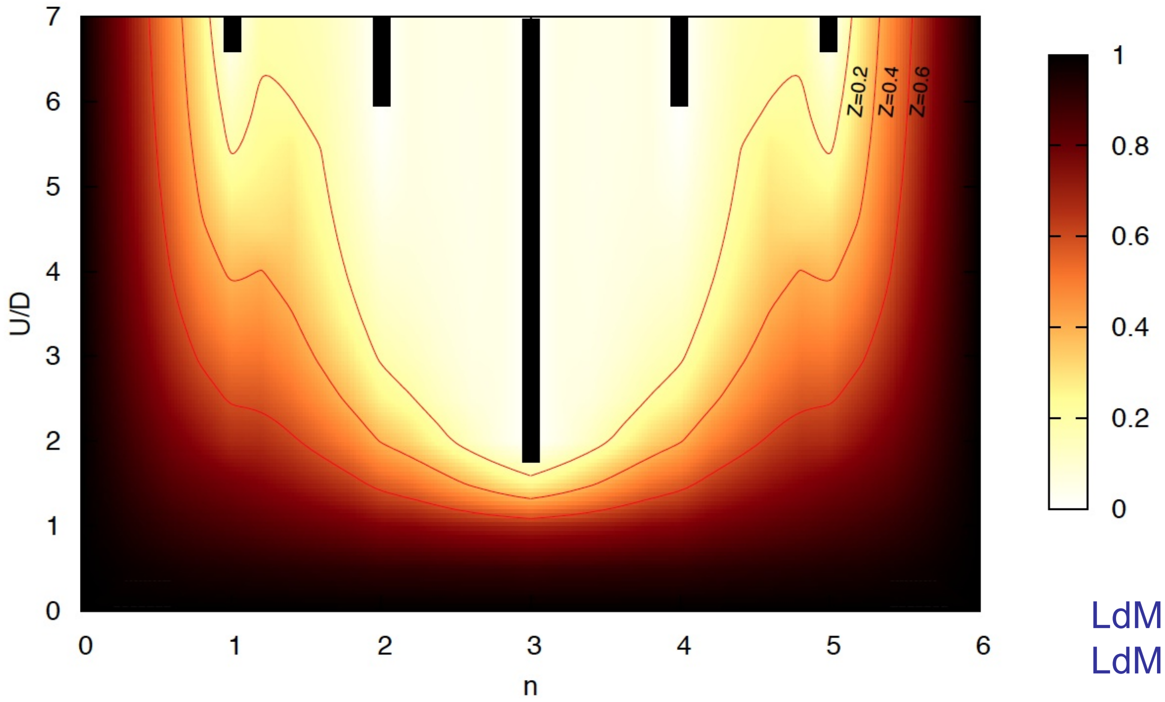
- half-filling: ~U+(N-1)J
- other filling: ~U-3J

LdM, PRB **83** (2011)
LdM, J. Mravlje, A. Georges, PRL **107** (2011)

Number N of electrons in M orbitals	Degeneracy of atomic ground-state	Mott gap	Correlations	Materials behaviour promoted by J
one electron or one hole ($N = 1, 2M - 1$)	unaffected	reduced	diminished	metallic
half-filled ($N = M$)	reduced	increased	increased	insulating
All other cases ($N \neq 1, M, 2M - 1$)	reduced	reduced	Conflicting effect (see text)	bad metallic

Table I: The effects of an increasing Hund's rule coupling on the degree of correlations.

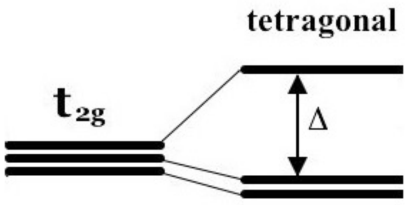
3 orbitals (relevant for t_{2g} materials)

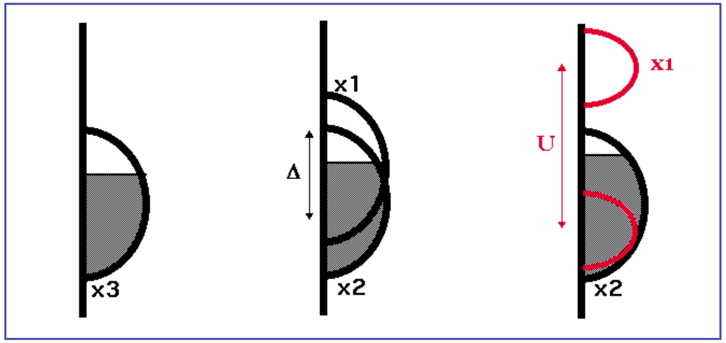


LdM, PRB **83** (2011)
LdM, J. Mravlje, A. Georges, PRL **107** (2011)

Number N of electrons in M orbitals	Degeneracy of atomic ground-state	Mott gap	Correlations	Materials behaviour promoted by J
one electron or one hole ($N = 1, 2M - 1$)	unaffected	reduced	diminished	metallic
half-filled ($N = M$)	reduced	increased	increased	insulating
All other cases ($N \neq 1, M, 2M - 1$)	reduced	reduced	Conflicting effect (see text)	bad metallic

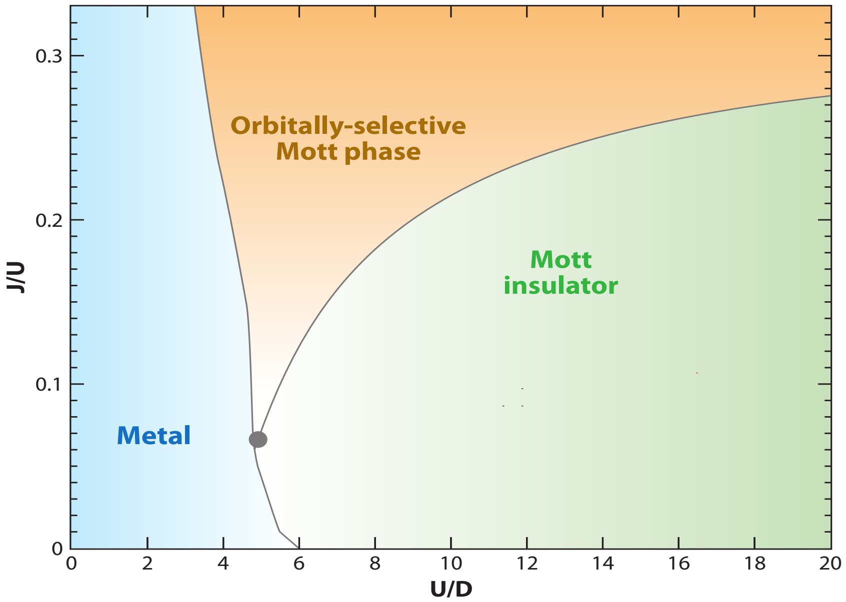
Table I: The effects of an increasing Hund's rule coupling on the degree of correlations.





3 bands of the same width

Crystal-field (one band up)
+ Hund's coupling



LdM, S.R. Hassan, M. Capone, X. Dai, PRL 102 (2009)

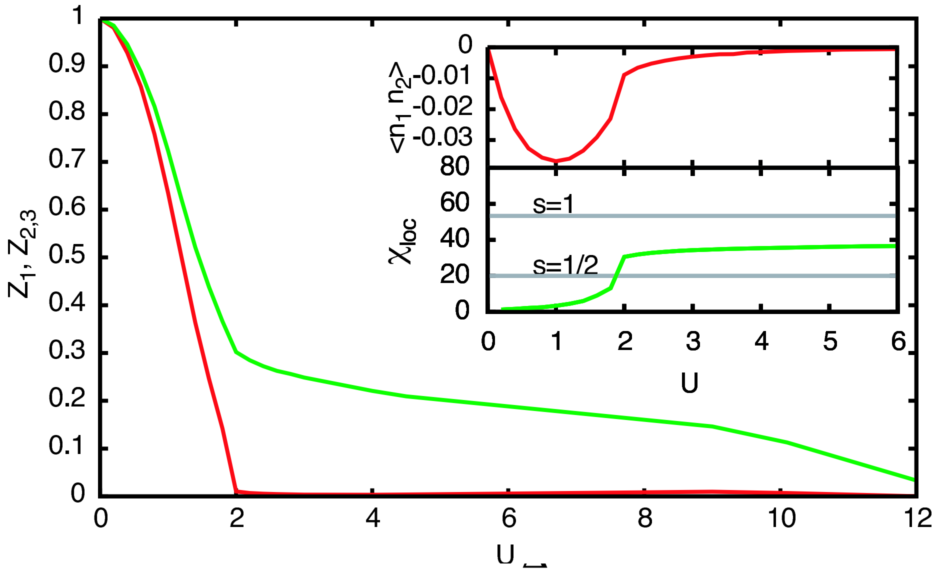
Orbital-selective Mott transition

- Coexisting itinerant and localized conduction electrons
- Metallic resistivity and free-moment magnetic response
- non Fermi-liquid physics of the intinerant electrons

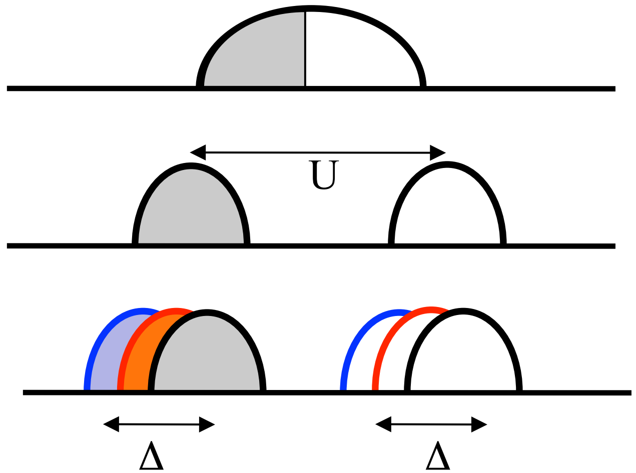
Anisimov et al., Eur. Phys. J. B 25 (2002)
Koga et al., Phys. Rev. Lett. 92 (2004)
For a review:
M. Vojta J. Low Temp. Phys. 161 (2010)

J favors the OSMT

Hund's coupling as an orbital decoupler



Hund's coupling acts as an **orbital-decoupler**



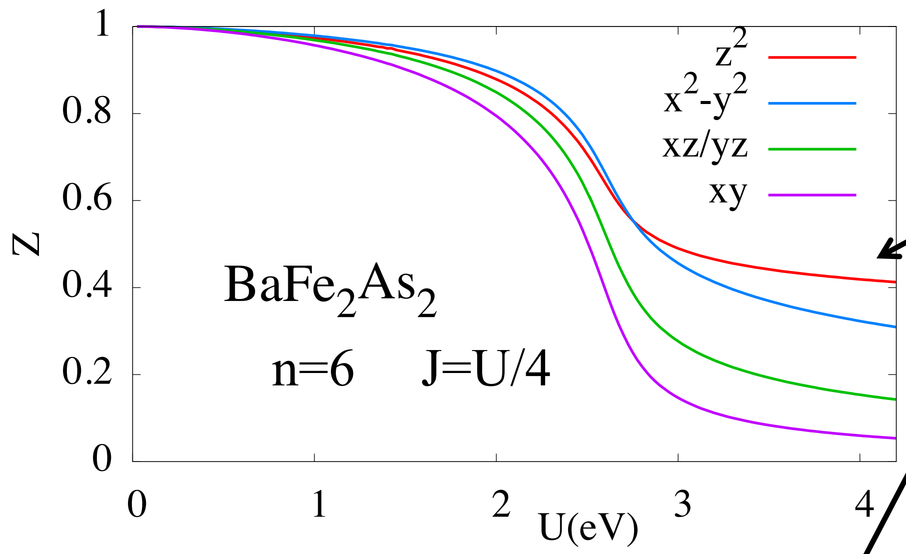
Crucial: Hund's coupling suppresses the orbital fluctuations, rendering the orbitals independent from one-another

(OSMT is the extreme case. More generally J favors a differentiation in the correlation strength for each orbital)

LdM, S.R. Hassan, M. Capone, X. Dai, PRL**102** (2009)
LdM, Phys. Rev. B **83** (2011)
Werner and Millis, Phys. Rev. Lett. **99** (2007)

DFT+Slave-spins: $BaFe_2As_2$

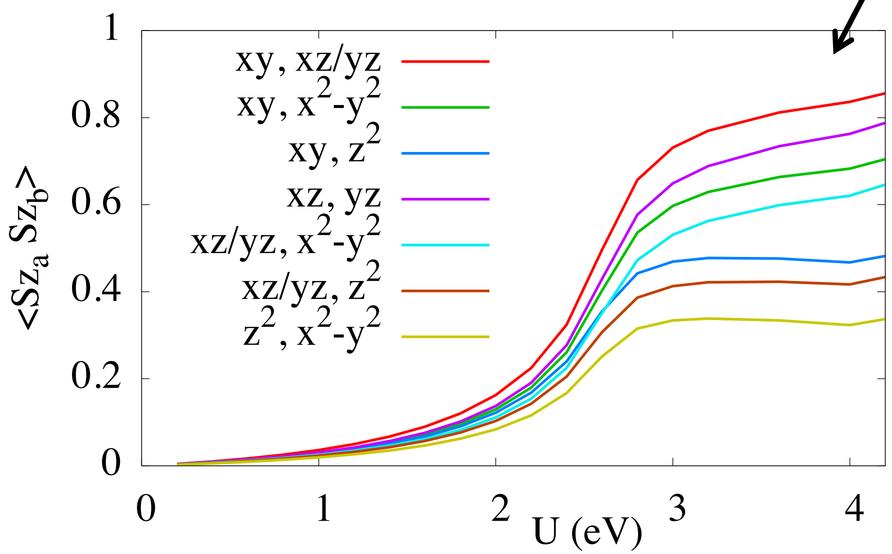
'Hund's metal'

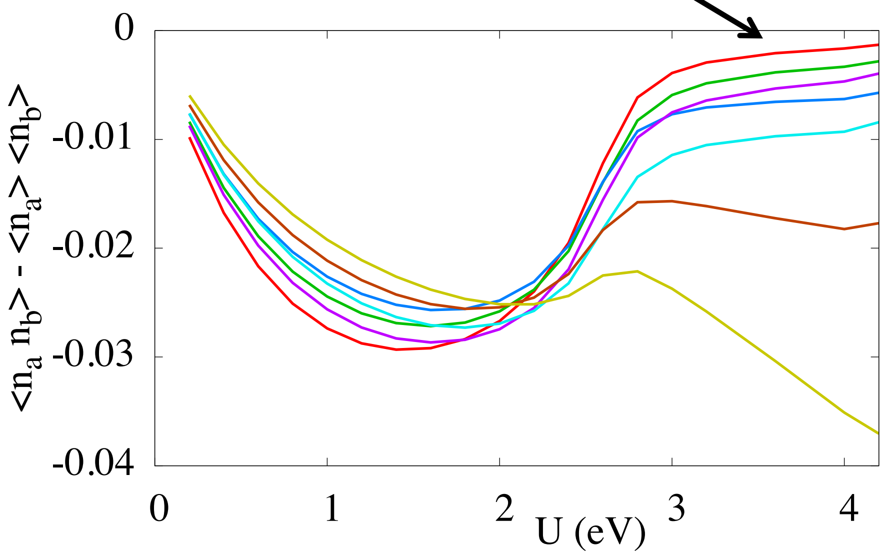


Janus behaviour

Interorbital spin correlations: locked spins

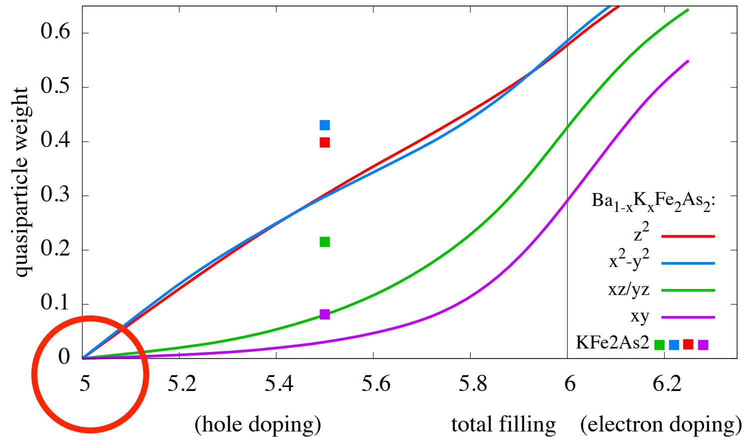
Interorbital charge correlations: suppressed



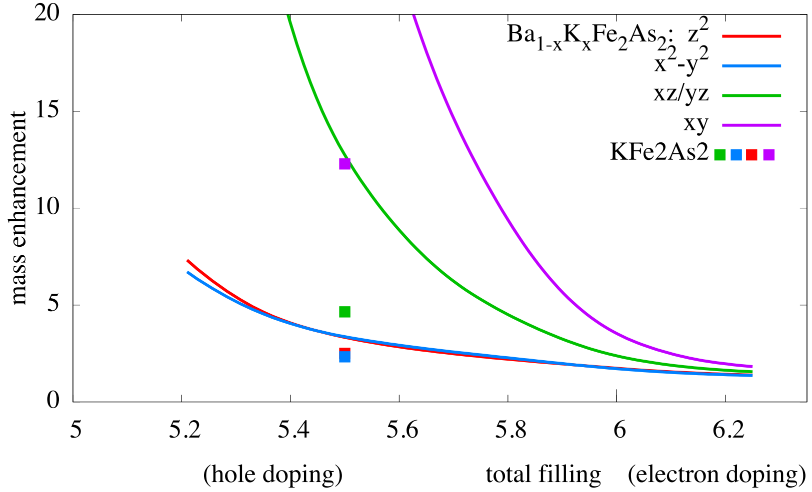


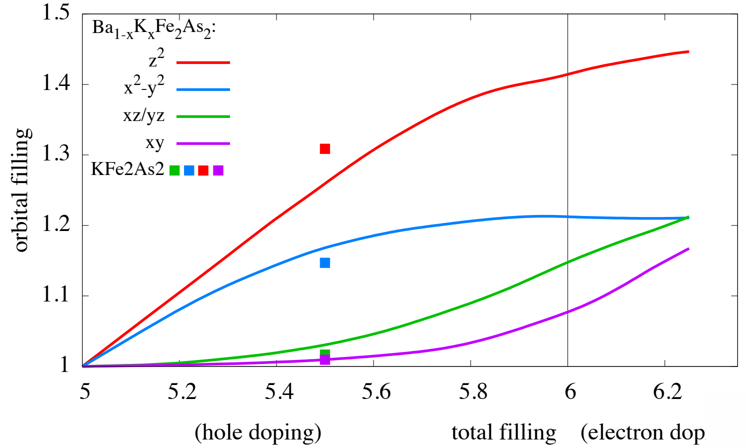
See also work by: Aichhorn et al, Craco, Laad et al, R. Yu and Q. Si, Lanatà et al., Yin et al, Bascones et al., …

Selective Mottness in iron-SC: doped BaFe2As2 (DFT+SSpins)

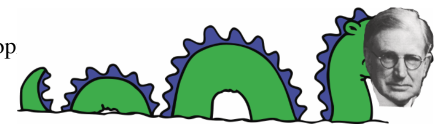


Mott Insulator





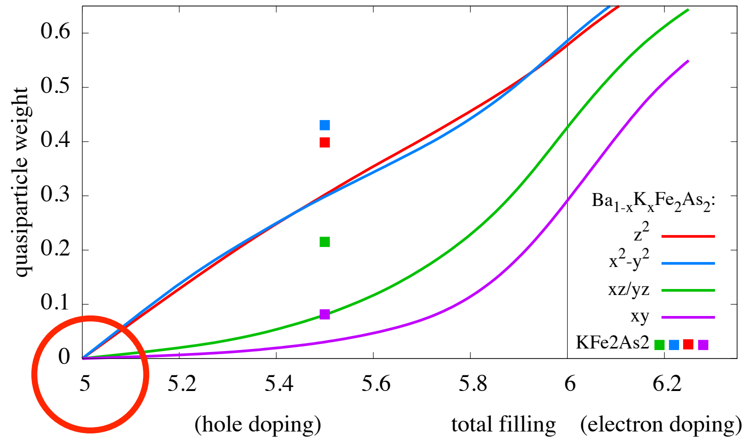
Strinking linear behaviour, when plotting Z against the individual orbital populations



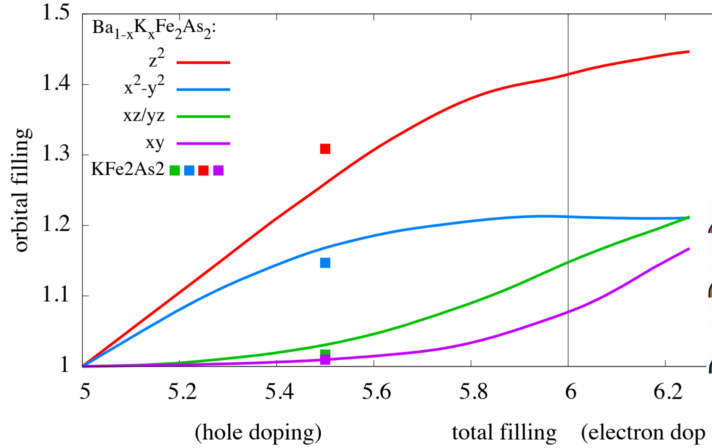
Mottness

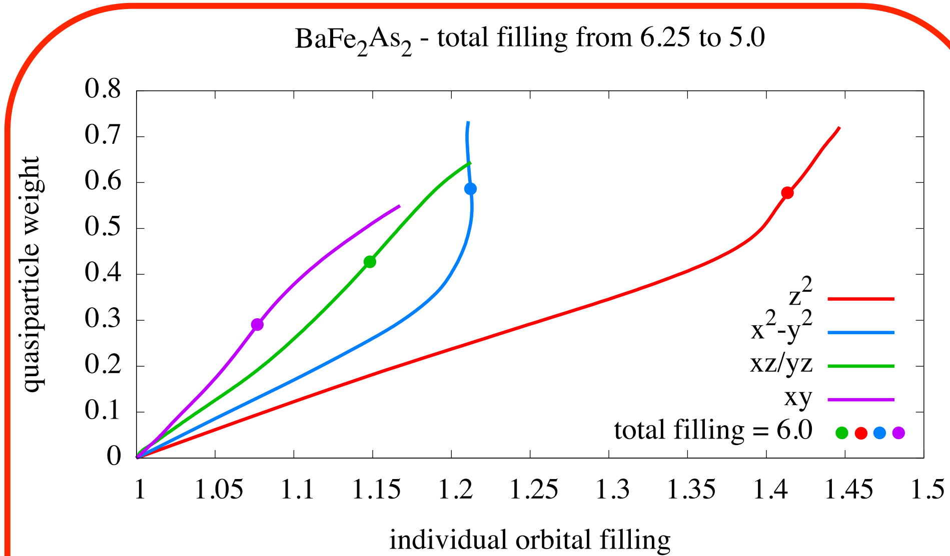
Similar evidences from
LDA+DMFT: Ishida et al., PRB **81** (2010)
Variational MC: Misawa et al.,PRL **108** (2012)

Selective Mottness in iron-SC: doped BaFe2As2 (DFT+SSpins)

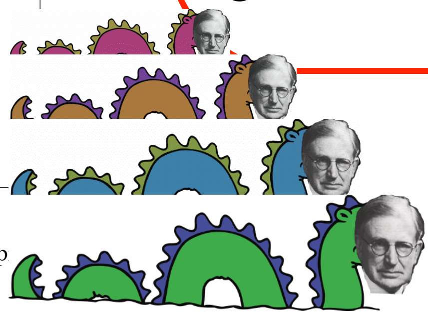


Mott Insulator





Strinking linear behaviour, when plotting Z against the individual orbital populations



Each orbital behaves as a doped Mott insulator

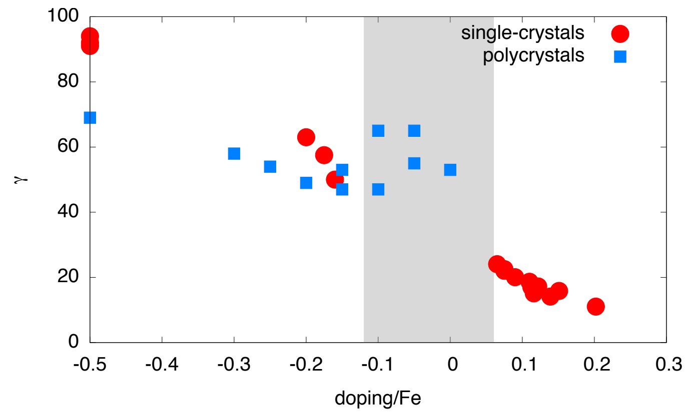
Selective Mottness!

<u>orbital decoupling</u>, and influence of the n=5 Mott insulator

Similar evidences from
LDA+DMFT: Ishida et al., PRB **81** (2010)
Variational MC: Misawa et al.,PRL **108** (2012)

Specific heat in Ba-122

Specific heat - single crystals			(1 this work)
doping/Fe	γ exp.	γ_b DFT	$m^*/m = \gamma/\gamma_b$
0.202	11.03 [3]	9.44 [1]	1.17
0.151	15.84 [3]	10.32 [1]	1.53
0.139	14.11 [3]	9.75 [1]	1.45
0.122	17.22 [3]	9.44 [1]	1.82
0.116	15.11 [3]	9.41 [1]	1.60
0.1125	17.02 [3]	9.41 [1]	1.80
0.11	18.67 [3]	9.38 [1]	1.99
0.09	20.06 [3]	10.12 [1]	1.98
0.075	22.02 [3]	10.96 [1]	2.0
0.075	22.53 [3]	10.96 [1]	2.05
0.065	24.06 [3]	11.03 [1]	2.18
-0.16	50 [4]	12.17 [1]	4.09
-0.175	57.5 [5]	12.00 [1]	4.66
-0.20	63 [6]	11.80 [1]	5.01
-0.5	91 [7]	10.1 [8]	9.0
-0.5	94 [9]	10.1 [8]	9.3



caveats:
- extrapolation to zero T
- substraction of phonon contribution
- poly vs single crystals

A strong mass enhancement for diminishing filling!

Optics		
doping/Fe	m^*/m (fit)	m^*/m (cutoffs)
0.18	1.48[15]	1.79[16]
0.11	1.98[15]	2.28[16]
0.061	4.21[15]	3.50[16]
0.051	4.56[15]	3.80[16]
0.025	4.78[15]	4.99[16]
0.0	3.3[13, 15]	4.80[16]
-0.2		3.31[17]
-0.225		3.15[18]
-0.5		3.37[19]

caveats:
- difficulty in isolating the Drude contribution(s)
-several Drude-Lorentz fits are possible
- interband transitions at low energy
- coupling to bosonic modes, etc

Indicative: overall moderate correlation strength

ARPES and quantum oscillations in Ba-122

Luca de' Medici

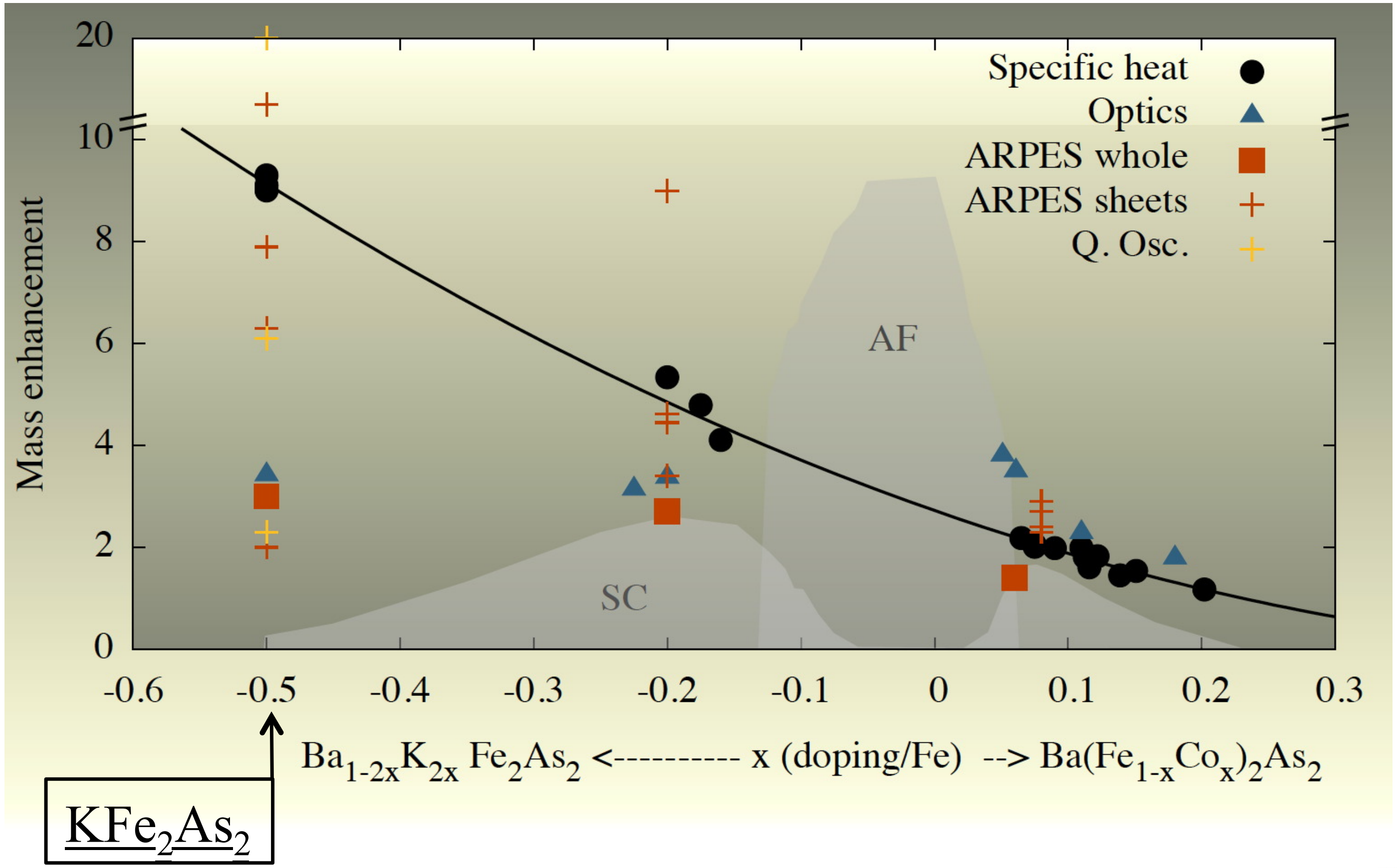
ARPES								
doping per Fe	whole	sheets					z^2 band	Ref.
		α	β	ζ	γ	δ/ϵ		
0.08		2.7	2.3		2.4	2.9		[21]
0.06	1.4							[22]
-0.2	2 (2.7[22])	3.4	4.45		4.62	9.0		[23]
-0.5	3	2.0	6.3	7.9		18.7	3	[24]
Quantum oscillations								
-0.5		2.3		6.1		20		[8]

caveats: energy shifts of the bands when comparing to DFT

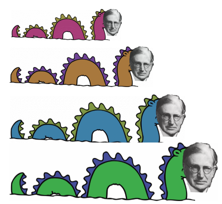
Correlations increase when reducing the filling and estimates for the different Fermi sheets spread more and more. Orbital selectivity!

Experimental mass enhancements

(high-T tetragonal phase)

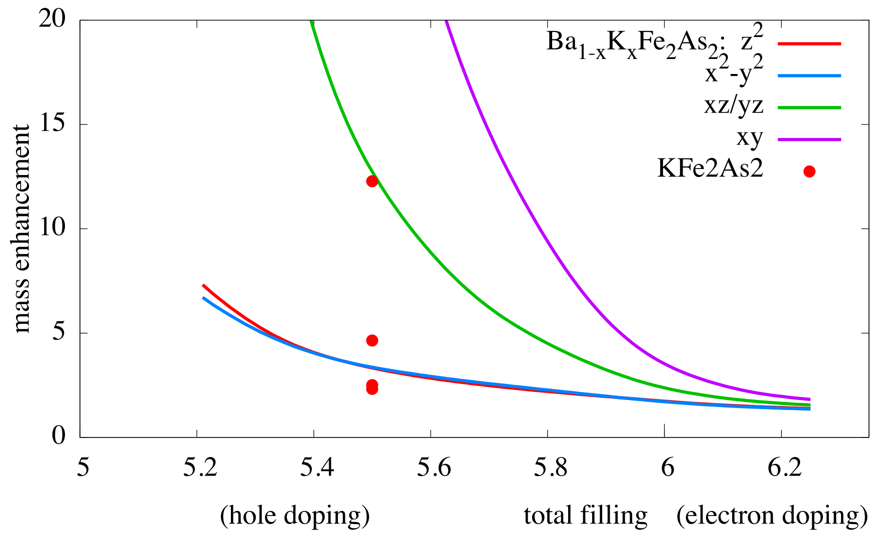


Strongly or weakly correlated? Both!
Selective Mottness confirmed!

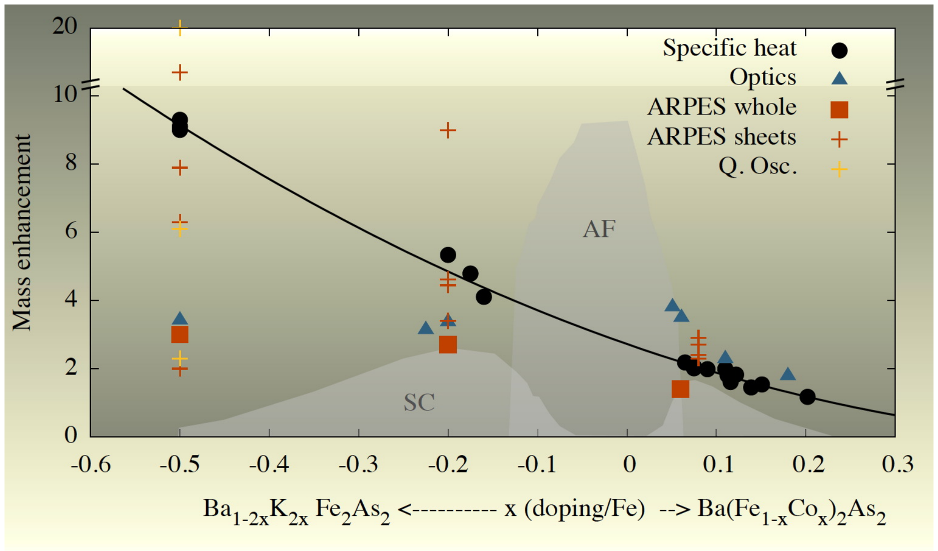


mass enhancements

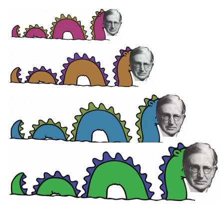
Theory



Experimental data

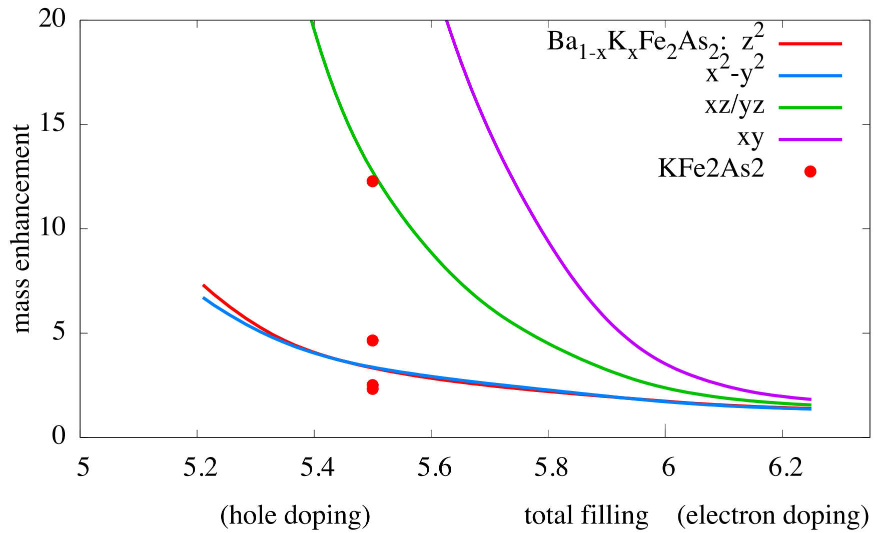


Strongly or weakly correlated? Both!
Selective Mottness confirmed!

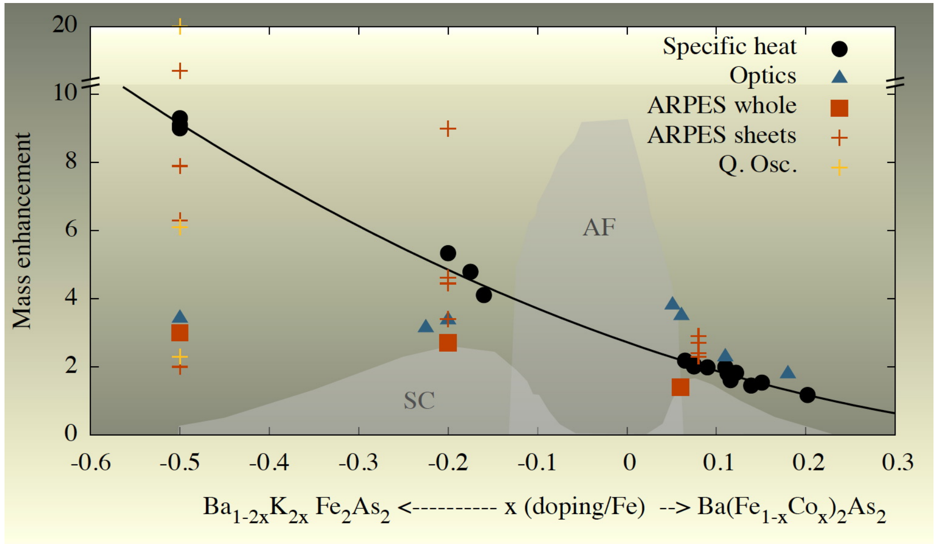


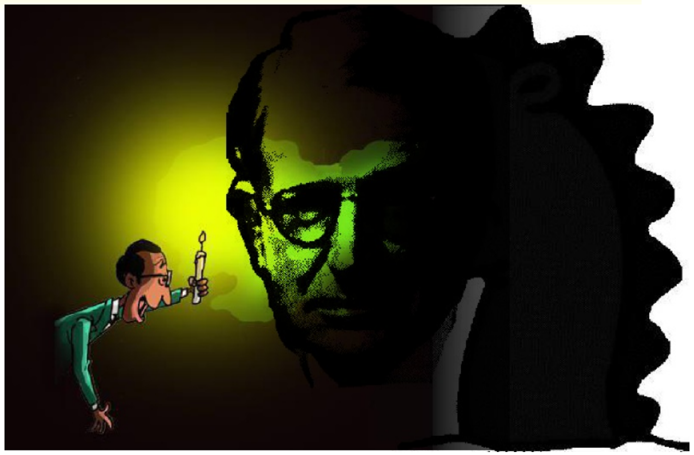
mass enhancements

Theory



Experimental data





Mott is near!!
(nearer for some orbitals)
Because of orbital decoupling

PRL **111,** 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

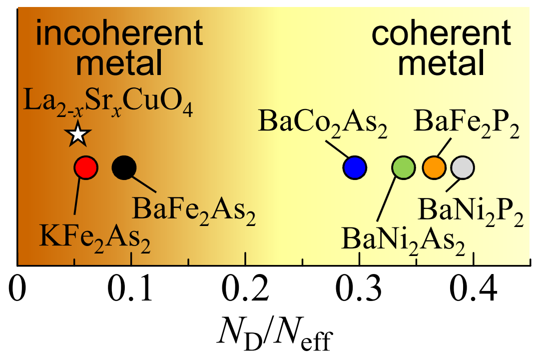
F. Hardy,[1,*] A. E. Böhmer,[1] D. Aoki,[2,3] P. Burger,[1] T. Wolf,[1] P. Schweiss,[1] R. Heid,[1] P. Adelmann,[1] Y. X. Yao,[4] G. Kotliar,[5] J. Schmalian,[6] and C. Meingast[1]

[1]*Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany*
[2]*INAC/SPSMS, CEA Grenoble, 38054 Grenoble, France*
[3]*IMR, Tohoku University, Oarai, Ibaraki 311-1313, Japan*
[4]*Ames Laboratory US-DOE, Ames, Iowa 50011, USA*
[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[6]*Karlsruher Institut für Technologie, Institut für Theorie der Kondensierten Materie, 76128 Karlsruhe, Germany*

(Received 15 January 2013; published 9 July 2013)

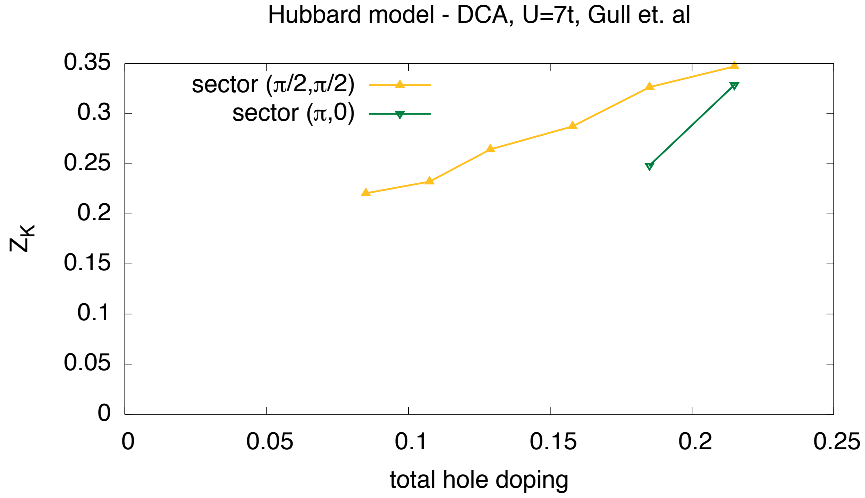
Using resistivity, heat-capacity, thermal-expansion, and susceptibility measurements we study the normal-state behavior of KFe_2As_2. Both the Sommerfeld coefficient ($\gamma \approx 103$ mJ mol^{-1} K^{-2}) and the Pauli susceptibility ($\chi \approx 4 \times 10^{-4}$) are strongly enhanced, which confirm the existence of heavy quasiparticles inferred from previous de Haas–van Alphen and angle-resolved photoemission spectroscopy experiments. We discuss this large enhancement using a Gutzwiller slave-boson mean-field calculation, which shows the proximity of KFe_2As_2 to an orbital-selective Mott transition. The temperature dependence of the magnetic susceptibility and the thermal expansion provide strong experimental evidence for the existence of a coherence-incoherence crossover, similar to what is found in heavy fermion and ruthenate compounds, due to Hund's coupling between orbitals.

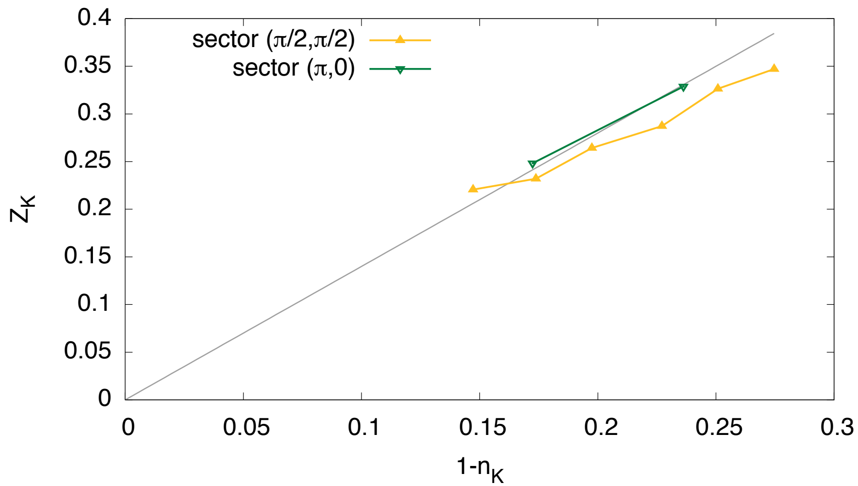
Nakajima et al. ArXiv:1308.6113

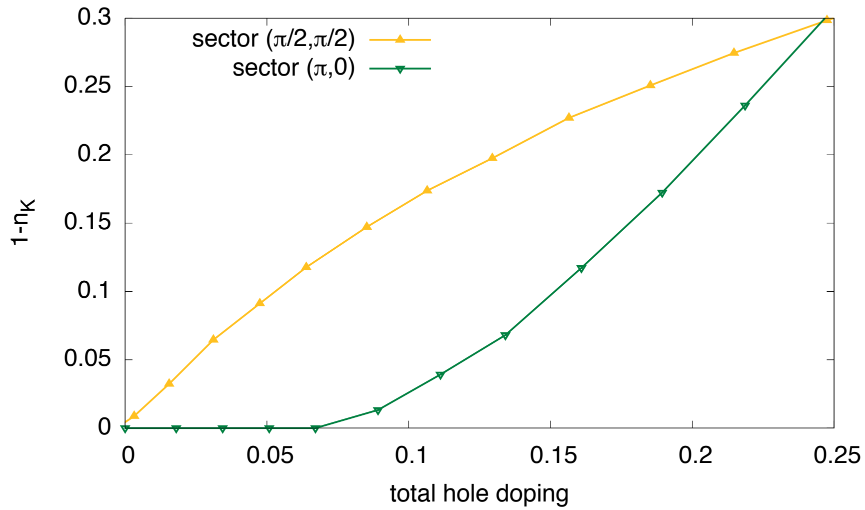


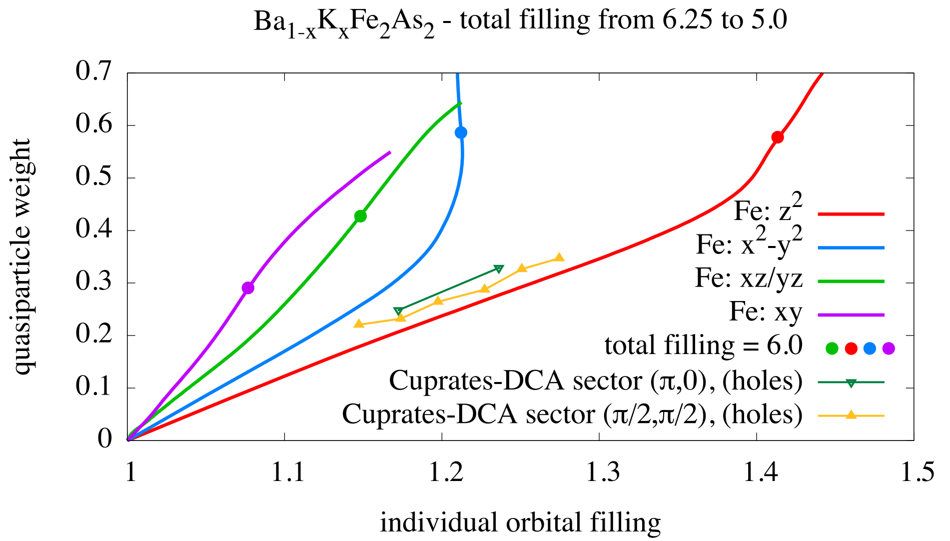
Cuprates: DCA approach to the 2D Hubbard model

Luca de' Medici

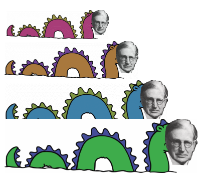






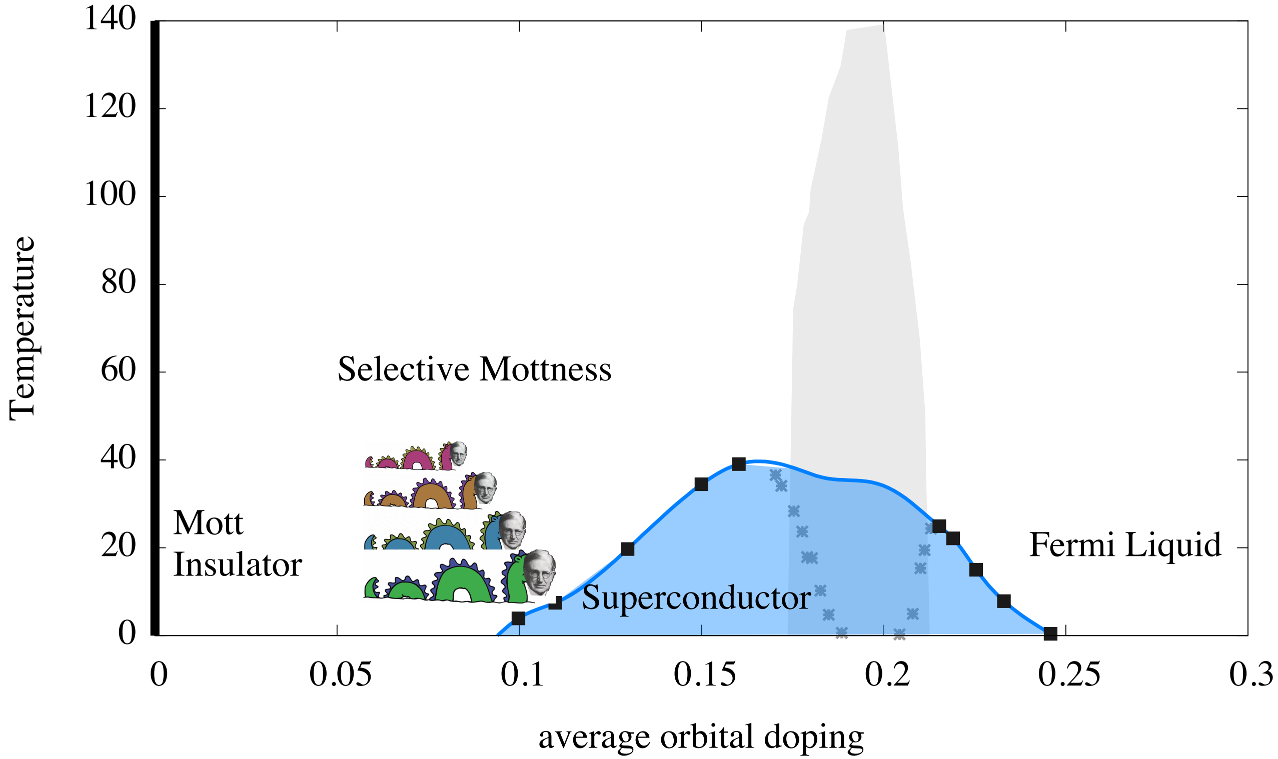


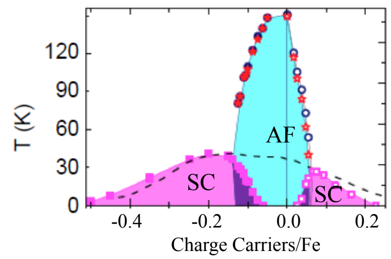
Data from: Gull et al.
Phys Rev. B 82, 155101 (2010)

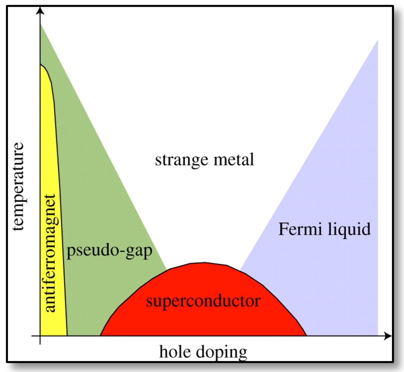


Same orbital decoupling!

Tentative common phase diagram for Cuprates and Iron-SC







When plotted against the average orbital doping the experimental phase diagram of iron-SC closely resembles the one for cuprates! (suppressing magnetism)

- a superconducting dome at 20% doping from a Mott insulator
- a phase with selective Mottness in between the two
- a good Fermi-liquid at higher dopings

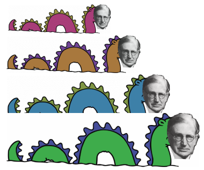
Is then **selective Mottness important for superconductivity?**

A. Hackl and M. Vojta, New J. Phys.11 (2009)
Kou et al. Europhys. Lett. 88 (2009)
Yin W-G et al. Phys. Rev. Lett. 105 (2010)
You Y-Z et al., Phys. Rev. Lett.107 (2011)

Conclusions:

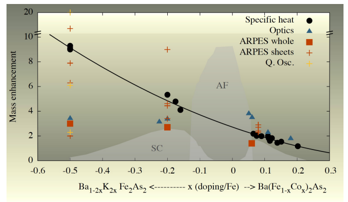
A guide from theory: Hund's has a key-role in tuning correlations in 3d materials

- Conduction-band filling is the key variable: Mott insulators are favored at half-filling, 'bad-metals' at neighboring filling
- J acts as an "**orbital-decoupler**" and favors **orbital selective Mottness**

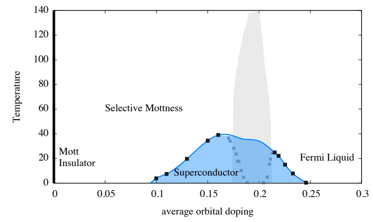


In Iron Superconductors:

- makes them **correlated**, even if far from the n=6 Mott insulating state (Janus effect). A Mott insulator would be realized at n=5!
- Induces **selective Mottness**, i.e. coexistence of strongly and weakly correlated electrons



A common phase diagram with cuprates?



LdM, S.R. Hassan, M. Capone, X. Dai, PRL **102**, 126401 (2009)
LdM, S.R. Hassan, M. Capone, JSC **22**, 535 (2009)
LdM, PRB **83**, 205112 (2011)
LdM, J. Mravlje, A. Georges, PRL **107**, 256401 (2011)
A. Georges, LdM, J. Mravlje, Annual Reviews Cond. Mat. 4, 137 (2013)
LdM, G. Giovannetti, M. Capone, 'Selective Mottness as a key to Iron superconductors' (ArXiv:1212.3966)

Acknowledgements:
G. Giovannetti and M. Capone, E. Winograd